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Hopping transport equation for electrons in superlattices with vertical disorder

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Abstract. We develop a theory of vertical hopping transport in doped superlattices with intentional vertical disorder introduced by controlled random variations of well widths. For structures with sufficiently large disorder, the vertical conductance (in the direction of the growth axis) is limited by phonon-assisted hopping between the wells. It is shown that due to quasi-equilibrium situation within the wells, the master rate equation for transitions between the electronic states of the structure can be reduced to a truncated rate equation for inter-well transitions only. At low bias, the solution of this rate equation is shown to be equivalent to finding total resistance of a quasi-one-dimensional network of resistances expressed in terms of integral transition rates between the wells. This network is generally different from the Miller–Abrahams network and contains multisite resistors.

Introduction

Superlattices with intentional disorder (SLIDs) in which vertical disorder (in the direction of the growth axis) was introduced by random controlled variations of well widths in the process of structure deposition were first discussed in [1] and were experimentally realized in [2]; vertical transport in such structures was studied both by optical methods, in particular, by stationary and picosecond luminescence spectroscopy (e.g., see [2]), and by direct measurements of the vertical conductance [3]. Optical experiments clearly showed that with increasing vertical disorder, localization of electronic states in the direction of the structure growth increases. It was argued that for small overlap of the wave functions of neighboring wells even for superlattices without intentionally introduced disorder, vertical transport can be due to phonon-assisted inter-well transitions (hopping) [4, 5]. Introduction of intentional disorder substantially enhances localization of electronic states; for short-period superlattices GaAs/AlAs with random fluctuations of well and barrier widths (from 1 to 3 monolayers), the onset of localization was studied in [6]. At low energies, the decay length of the wave function can become smaller than the monolayer width so that structures considered seem to be similar to a one-dimensional chain of localized states. For structures with sufficiently large disorder studied in [3], the miniband width was estimated to be smaller than the width of the level distribution; therefore one expects that the states are strongly localized in the vertical direction. Thus it appears that vertical transport in SLIDs is similar to that in one-dimensional systems of localized states (sites), and SLIDs are very promising model systems to study the effects of disorder and Coulomb interactions on electronic states and transport. Indeed, phonon-assisted hopping for usual one-dimensional and quasi-one-dimensional of sites was extensively studied by using the quantum transport equation techniques and percolation theory (e.g., see [7, 8]); therefore, comparison of experimental data for SLIDs with localization and transport theories might appear to be a useful test of current theoretical concepts.

However, it recently became clear that there are essential differences between SLIDs and standard systems of point sites. In particular, it appears that a finite extent of the "cores" of

localized states in the vertical direction is important, giving rise to virtual-tunneling-assisted hopping [9] - [11]. Moreover, sites cannot be assigned to individual quantum states; one must rather associate sites with quantum wells, which are macroscopically populated. In this paper we discuss an approach that takes account of the specific natures of SLIDs, derive a truncated rate equation for macroscopic sites and establish the equivalence of the problem to that of a generalized resistance network.

1. Transport equation

As usual, in the envelope function approximation the wave functions of electronic states in SLIDs can be written in the form $\psi_{\lambda\mathbf{k}_\parallel} = Au_\lambda(z)\exp(i\mathbf{k}_\parallel\rho)$, where A is a normalizing factor, z is the coordinate in the SLID growth direction, $\mathbf{k}_\parallel$ and ρ are the in-plane position and momentum vectors, $u_\lambda(z)$ is the wave function for an eigenstate λ with energy ε_λ corresponding to the solution of the one-dimensional problem with the potential $V(z) = \sum_n V_n(z)$ describing the modulation of the conduction band edge, and $V_n(z)$ is the potential of the n th well. The energies of the states $\{\lambda\mathbf{k}_\parallel\}$ are $E_{\lambda\mathbf{k}_\parallel} = \epsilon_\lambda + \hbar^2k_\parallel^2/2m$. For the structures considered, typical well widths are such that for a single-well problem, upper size quantization levels in the wells lie much higher than the lowest levels. Therefore, in what follows we neglect contributions from all dimensional subbands except the lowest one. For strong disorder, the states $\{\lambda\mathbf{k}_\parallel\}$ are strongly localized in the z-direction and the u_λ are close to the corresponding "atomic-like" wave functions with small admixture of wave functions of neighboring wells.

The quantum transport equation describing transition between the states $\{\lambda\mathbf{k}_\parallel\}$ has a form

$$\frac{df_{\lambda\mathbf{k}_\parallel}}{dt} = -\sum_{\lambda'\mathbf{k}'_\parallel}\left\{W_{\lambda'\mathbf{k}'_\parallel,\lambda\mathbf{k}_\parallel}f_{\lambda\mathbf{k}_\parallel}\left(1-f_{\lambda'\mathbf{k}'_\parallel}\right) - W_{\lambda\mathbf{k}_\parallel,\lambda'\mathbf{k}'_\parallel}f_{\lambda'\mathbf{k}'_\parallel}\left(1-f_{\lambda\mathbf{k}_\parallel}\right)\right\}, \qquad (1)$$

where $f_{\lambda\mathbf{k}_\parallel}$ is an average occupation number of the state $\{\lambda\mathbf{k}_\parallel\}$ and $W_{\lambda'\mathbf{k}'_\parallel,\lambda\mathbf{k}_\parallel}$ is the probability of transitions from the state $\{\lambda\mathbf{k}_\parallel\}$ to $\{\lambda'\mathbf{k}'_\parallel\}$. Equation (1) contains both intra- and interwell transitions. If we neglect interwell transitions, we arrive at a system of standard independent Boltzmann transport equations; each of these describes transport and relaxation in the corresponding well. Since we are not interested in transport along the well planes, we do not write out explicitly intrawell diffusion and drift terms.

We show that Eq. (1) can be reduced to a truncated rate equation that contains only interwell transition rates. To this end, we sum both sides of Eq. (1) over $\mathbf{k}_\parallel$:

$$\frac{dv_\lambda}{dt} = -S^{-1}\sum_{\mathbf{k}_\parallel,\mathbf{k}'_\parallel,\lambda'\neq\lambda}\left\{W_{\lambda'\mathbf{k}'_\parallel,\lambda\mathbf{k}_\parallel}f^{(qe)}_{\lambda\mathbf{k}_\parallel}\left(1-f^{(qe)}_{\lambda'\mathbf{k}'_\parallel}\right) - W_{\lambda\mathbf{k}_\parallel,\lambda'\mathbf{k}'_\parallel}f^{(qe)}_{\lambda'\mathbf{k}'_\parallel}\left(1-f^{(qe)}_{\lambda\mathbf{k}_\parallel}\right)\right\}, \qquad (2)$$

where $v_\lambda = S^{-1}\sum_{\mathbf{k}_\parallel} f^{(qe)}_{\lambda\mathbf{k}_\parallel}$ are nonequilibrium aerial concentrations, $f^{(qe)}_{\lambda\mathbf{k}_\parallel}$ are the local quasi-equilibrium (quasi-Fermi) distributions characterized by the quasi-Fermi levels μ_λ and S is the structure area. In Eq. (2) the intrawell transitions canceled out. Moreover, since for the structures considered the intrawell transition rates are much greater than those of interwell transitions, a "local" equilibrium is established in each of the wells, and the functions $f_{\lambda\mathbf{k}_\parallel}$ in the interwell transition rates can be replaced by $f^{(qe)}_{\lambda\mathbf{k}_\parallel}$. Thus Eq. (2) is considerably simpler than the master equation (2), since it contains no intrawell transition rates.

2. Linear theory and resistance network

Now let an electric field be applied in the direction of the z-axis; for states strongly localized in the z-direction, its effect can be described by the corresponding energy shifts $\epsilon_\lambda \to \epsilon_\lambda + U_\lambda$, where U_λ is the potential energy at the localization region of the state λ. An applied field generally produces variations of carrier concentrations in the wells related to the shifts of local quasi-Fermi levels $\delta\mu_\lambda$. Just as in the standard hopping theory [8], we can linearize Eq. (2) taking account of the fact that transition probabilities $W_{\lambda\mathbf{k}_\parallel,\lambda'\mathbf{k}'_\parallel}$ are energy-dependent. Then we arrive at the linearized equation

$$\frac{dv_\lambda}{dt} = \frac{1}{SkT}\sum_{\lambda'\neq\lambda}\Gamma_{\lambda,\lambda'}(U_\lambda + \delta\mu_\lambda - U'_\lambda - \delta\mu'_\lambda), \tag{3}$$

where the "integral" transition rates are

$$\Gamma_{\lambda,\lambda'} = \sum_{\mathbf{k}_\parallel,\mathbf{k}'_\parallel} W_{\lambda\mathbf{k}_\parallel,\lambda'\mathbf{k}'_\parallel} f^{(0)}_{\lambda\mathbf{k}_\parallel}\left(1 - f^{(0)}_{\lambda'\mathbf{k}'_\parallel}\right), \tag{4}$$

the transition probabilities are taken with unshifted energies and $f^{(0)}_{\lambda\mathbf{k}_\parallel}$ are the equilibrium (Fermi) distribution.

Equation (4) is similar to the standard linearized hopping rate equation [8] with some important differences. First, the sites here are not single-electron states but rather multi-electron: they can be related to "macroscopic" quantum wells that contain many electrons. It follows that correlation effects such as Hubbard repulsion and Coulomb gap effects are expected to be much weaker than in standard hopping problems. Second, the transition rates $\Gamma_{\lambda,\lambda'}$ are integral rates obtained by summing over the initial and final states of the wells with different $\mathbf{k}_\parallel$ and $\mathbf{k}'_\parallel$.

It follows from Eq. (2) that just as in the standard hopping theory [7, 8, 12], the low-field problem can be reduced to an equivalent resistance network; in our case the resistances $R_{\lambda\lambda'}$ between the states λ and λ' are expressed in terms of the integral rates by $R^{-1}_{\lambda\lambda'} = (e/SkT)\Gamma_{\lambda,\lambda'}$.

3. Discussion

It should be noted that for weak overlap of wave functions of neighboring wells and strong disorder, instead of the eigenstates $\{\lambda\mathbf{k}_\parallel\}$, we can use a basis of "atomic-like" wave functions $\phi_n(z)$ localized at the corresponding wells n; in this case one can associate the sites of the resistance network with the wells. It was shown in [9, 10] that for sites with finite-size cores, hybridization effects can be important even for small overlap. In this case the interwell transition probabilities depend on parameters (in particular, on energies) of intermediate virtual states, and network resistances are no more reduced to two-well resistances $R_{nn'}$ but are "multisite". Moreover, hybridized (cluster) states corresponding to different energies can include different sites and, on the other hand, the same site can belong to different cluster states, i.e., different multisite resistances can "overlap".

In some cases (e.g., for nearest-neighbor hopping or for systems with sufficiently large disorder) the complicated structure of the network is not crucial for the calculation of the total network resistance. In fact, if the total resistance is determined by the resistance of the critical region, percolation arguments hold, and the network resistance can be evaluated in a straightforward way [9, 10].

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